Anisole

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 7.33e-01 mol/L

Global applicability domain: Inside

Local applicability domain index: 6.26e-01

Confidence level: 6.08e-01

Nearest Neighbors from the Training Set

Image not found
1-Propene, 3,3'-oxybis-
Measured: 9.54e-01
Predicted: 6.49e-01

Image not found
Cyclohexylamine
Measured: 10.1
Predicted: 5.21

Image not found
2-Methyltetrahydrofuran
Measured: 1.81
Predicted: 9.09e-01

Image not found
Cyclopropane, ethoxy- (9CI)
Measured: 2.29e-01
Predicted: 6.72e-01